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Differential Transformation Method for a Reliable Treatment of the Nonlinear Biochemical Reaction Model

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Abstract

In this paper, we present a numeric-analytic solution of the well-known Michaelis–Menten nonlinear biochemical reaction system based on differential transformation method (DTM). We shall compare the DTM against the homotopy-perturbation method (HPM). The numerical results obtained from the DTM and HPM are in complete agreement.

Keywords: Differential transformation method; Taylor's series expansion, nonlinear biochemical reaction model

1 Introduction

The concept of differential transformation method was first proposed by Zhou [1] in 1986 (see [2, 3]), and it was applied to solve linear and non-linear initial value problems in electric circuit analysis. This method constructs a semi-analytical numerical technique that uses Taylor series for the solution of differential equations in the form of a polynomial. It is different from the high-order Taylor series method which requires symbolic computation of the necessary derivatives of the data functions. The Taylor series method is computationally time-consuming especially for high order equations. The differential transform is an iterative procedure for obtaining analytic Taylor series solutions of differential equations. The Differential transformation method is very effective and powerful for solving various kinds of differential equations. For example, it was applied to two point boundary value problems [4], to differential-algebraic

equations [5], to the KdV and mKdV equations [6], to the Schrödinger equations [7], to fractional differential equations [8] and to the Riccati differential equation [9]. Jang *et al.* [10] introduced the application of the concept of the differential transformation of fixed grid size to approximate solutions of linear and non-linear initial value problems. Hassan [11] applied the differential transformation technique of fixed grid size to solve the higher-order initial value problems. The transformation method can be used to evaluate the approximating solution by the finite Taylor series and by an iteration procedure described by the transformed equations obtained from the original equation using the operations of differential transformation. The main advantage of this method is that it can be applied directly to linear and nonlinear ODEs without requiring linearization, discretization or perturbation. Another important advantage is that this method is capable of greatly reducing the size of computational work while still accurately providing the series solution with fast convergence rate.

In this paper, we consider Michaelis–Menten biochemical reaction model [12]



where E is the enzyme, A the substrate, Y the intermediate complex and X the product. The time evolution of scheme (1) can be determined from the solution of the system of coupled nonlinear ODEs

$$\frac{dA}{dt} = -k_1EA + k_{-1}Y, \quad (2)$$

$$\frac{dE}{dt} = -k_1EA + (k_{-1} + k_2)Y, \quad (3)$$

$$\frac{dY}{dt} = k_1EA - (k_{-1} + k_2)Y, \quad (4)$$

$$\frac{dX}{dt} = k_2Y, \quad (5)$$

subject to the initial conditions:

$$A(0) = A_0, \quad E(0) = E_0, \quad Y(0) = Y_0, \quad X(0) = X_0, \quad (6)$$

where the parameters k_1, k_{-1} and k_2 are positive rate constants for each reaction. Systems (2)–(5) can be reduced to only two equations for A and Y and in dimensionless form of concentrations of substrate, x , and intermediate complex between enzyme and substrate, y , are given by [13]

$$\frac{dx}{dt} = -x + (\beta - \alpha)y + xy, \quad (7)$$

$$\frac{dy}{dt} = \frac{1}{\epsilon}(x - \beta y - xy), \quad (8)$$

subject to initial conditions:

$$x(0) = 1, \quad y(0) = 0, \quad (9)$$

where α, β and ϵ are dimensionless parameters.

In this paper, we present a reliable algorithm based on DTM to find numeric-analytic solution of the system of coupled nonlinear ODEs (7) and (8).

2 The differential transformation method (DTM)

An arbitrary function $f(x)$ can be expanded in Taylor series about a point $x = 0$ as

$$f(x) = \sum_{k=0}^{\infty} \frac{x^k}{k!} \left[\frac{d^k f}{dx^k} \right]_{x=0}. \quad (10)$$

The differential transformation of $f(x)$ is defined as

$$F(x) = \frac{1}{k!} \left[\frac{d^k f}{dx^k} \right]_{x=0}. \quad (11)$$

Then the inverse differential transform is

$$f(x) = \sum_{k=0}^{\infty} x^k F(k). \quad (12)$$

The fundamental mathematical operations performed by differential transform method are listed in Table 1.

2.1 The operation properties of differential transformation

If $x(t), y(t)$ are two uncorrelated functions with time t and $X(k), Y(k)$ are the transformed functions corresponding to $x(t), y(t)$ and the basic properties are shown as follows:

1. If $X(k) = D[x(t)]$, $Y(k) = D[y(t)]$, and c_1 and c_2 are independent of t and k , then $D[c_1x(t) + c_2y(t)] = c_1X(k) + c_2Y(k)$.
(Symbol D denoting the differential transformation process).

Table 1: The fundamental operations of differential transformation method (DTM)

Original function	Transformed function
$y(x) = g(x) \pm h(x)$	$Y(k) = G(k) \pm H(k)$
$y(x) = \alpha g(x)$	$Y(k) = \alpha G(k)$
$y(x) = \frac{dg(x)}{dx}$	$Y(k) = (k + 1)G(k + 1)$
$y(x) = \frac{d^2g(x)}{dx^2}$	$Y(k) = (k + 1)(k + 2)G(k + 2)$
$y(x) = \frac{d^m g(x)}{dx^m}$	$Y(k) = (k + 1)(k + 2) \dots (k + m)G(k + m)$
$y(x) = 1$	$Y(k) = \delta(k)$
$y(x) = x$	$Y(k) = \delta(k - 1)$
$y(x) = x^m$	$Y(k) = \delta(k - m) = \begin{cases} 1, & k = m \\ 0, & k \neq m \end{cases}$
$y(x) = g(x)h(x)$	$Y(k) = \sum_{m=0}^k H(m)G(k - m)$

2. If $z(t) = x(t)y(t)$, $x(t) = D^{-1}[X(k)]$, $y(t) = D^{-1}[Y(k)]$ and \otimes denote the convolution, then
 $D[z(t)] = D[x(t)y(t)] = X(k) \otimes Y(k) = \sum_{r=0}^k Y(r)X(k - r)$.

3. If $y(x) = y_1(x)y_2(x) \dots y_{n-1}(x)y_n(x)$ then

$$Y(k) = \sum_{k_{n-1}=0}^k \sum_{k_{n-2}=0}^{k_{n-1}} \dots \sum_{k_2=0}^{k_3} \sum_{k_1=0}^{k_2} Y_1(k_1)Y_2(k_2 - k_1) \dots Y_{n-1}(k_{n-1} - k_{n-2})Y_n(k - k_{n-1}).$$

3 Application

By using the fundamental operations of differential transformation method in Table 1, we obtained the following recurrence relation to the system (7) and (8):

$$X(k + 1) = \frac{1}{(k + 1)} \left[-X(k) + \beta Y(k) - \alpha Y(k) + \sum_{m=0}^k X(m)Y(k - m) \right] \quad (13)$$

$$Y(k + 1) = \frac{1}{(k + 1)} \left[\frac{1}{\epsilon} X(k) - \frac{\beta}{\epsilon} Y(k) - \frac{1}{\epsilon} \sum_{m=0}^k X(m)Y(k - m) \right]. \quad (14)$$

From the initial condition $x(0) = 1$, $y(0) = 0$ we have $X(0) = 1$, $Y(0) = 0$, and from equations (13) and (14) and for the case $\alpha = 0.375, \beta = 1.0$ and

$\epsilon = 0.1$ we have

$$X(0) = 1, \quad X(1) = -1, \quad X(2) = \frac{69}{8}, \quad X(3) = \frac{-757}{12}, \quad X(4) = \frac{47767}{128}, \quad \dots(15)$$

$$Y(0) = 0, \quad Y(1) = 10, \quad Y(2) = -105, \quad Y(3) = \frac{9145}{12}, \quad Y(4) = \frac{-17785}{4}, \quad \dots(16)$$

Therefore, the closed form of the solution can be easily written as

$$x(t) = \sum_{k=0}^{\infty} X(k)t^k = 1 - t + \frac{69}{8}t^2 - \frac{757}{12}t^3 + \frac{47767}{128}t^4 - \frac{3800401}{1920}t^5 + \dots(17)$$

$$y(t) = \sum_{k=0}^{\infty} Y(k)t^k = 10t - 105t^2 + \frac{9145}{12}t^3 - \frac{17785}{4}t^4 + \frac{4440661}{192}t^5 + \dots(18)$$

The above results are in complete agreement with the results obtained by the homotopy perturbation method (HPM) reported in [14].

4 Conclusions

In this paper, we presented a reliable treatment based on the DTM to solve the well-known Michaelis–Menten nonlinear reaction system. The DTM was used in a direct way without using linearization, perturbation or restrictive assumptions. This method, unlike most numerical techniques, provides a closed-form solution. We conclude that the DTM is a promising tool for solving nonlinear systems of ODE.

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